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AN EFFICIENT FINITE DIFFERENCE SCHEME FOR THREE-DIMENSIONAL, NON-EQUILIBRIUM FLOWS USING OPERATOR SPLITTING

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Abstract—An efficient finite difference scheme is presented for the inviscid terms of the three-dimensional, compressible flow equations for chemical non-equilibrium gases. This scheme represents an extension and an improvement of one proposed by the author, and includes operator splitting.

1. INTRODUCTION

Recently [1] an approximate Riemann solver was presented for treating one-dimensional, inviscid, chemically reacting flows. The scheme in [1] represents an extension of one for flows in chemical equilibrium [2], and uses numerical characteristic decomposition, along the lines of that used in [2], for the more general flux terms arising in non-equilibrium flow. In addition to this, a stiff solver was suggested as a means of treating the source terms arising in the decoupled, scalar equations. An integral part of both the schemes in [1] and [2] is the special averages of flow variables required to make shock-capturing automatic. In particular, approximations are required for the derivatives of the equation of state in each computational cell.

The purpose of the present paper is two fold. Firstly, we present the corresponding results for the three-dimensional case which includes averages for the larger set of associated eigenvalues and eigenvectors, together with the use of operator splitting via the method of fractional steps [3]. Similar techniques have been used by other authors for non-equilibrium flows, (see e.g. [4]). Secondly, we make improvements on the approximations to the derivatives of the equation of state originally proposed in [1] and mentioned above. Improvements are made in two ways:

(1) the scheme presented here is more efficient than the original one in respect of the number of function evaluations of the equation of state that are required; and
(2) the modified scheme is more robust in the sense that no new, artificial states are introduced, unlike in the original scheme.

Both these points are explained in more detail in §4 following the three-dimensional form of the scheme in §3.

As stated in [1], we concentrate only on the modelling of the flux terms since the source terms can vary according to the chemical model of the production of species, in particular the number of reaction steps chosen, and the corresponding numerical treatment will generally be via an appropriate stiff-solver. Importantly, it is a straightforward matter to adapt existing codes based on the work in [1] to model the more general flux terms that arise in three dimensions, together with the modification mentioned above.

2. EQUATIONS OF FLOW

2.1 Equations of motion

The three-dimensional equations for the flow of an inviscid, compressible, chemically reacting fluid can be written in conservation form (with a source term) as

$$\underset{\sim}{w}_t + \underset{\sim}{f}_x + \underset{\sim}{g}_y + \underset{\sim}{h}_z = \underset{\sim}{s} \tag{2.1a}$$

where

$$\underset{\sim}{w} = (\rho_1, \rho_2, \ldots, \rho_{ns}, m, n, o, e)^T \tag{2.1b}$$

$$\underset{\sim}{f}(\underset{\sim}{w}) = \left(c_1 m, c_2 m, \ldots, c_{ns} m, m^2/\rho + p, mn/\rho, mo/\rho, m(e+p)/\rho\right)^T \tag{2.1c}$$

and

$$\underset{\sim}{s}(\underset{\sim}{w}) = (s_1, s_2, \ldots, s_{ns}, 0, 0)^T, \tag{2.1d}$$

with similar expressions for $\underset{\sim}{g}(\underset{\sim}{w})$ and $\underset{\sim}{h}(\underset{\sim}{w})$. The variables ρ_k, c_k, u, v, w and e represent the density (mass concentration) of the kth species, the species mass fraction, the velocity in each of the three coordinate directions x, y, z and the total energy, respectively. Also, $\rho = \sum_{k=1}^{ns} \rho_k$ so that $c_k \rho = \rho_k$, where ns is the number of species in the model, since $\sum_{k=1}^{ns} c_k = 1$. The global momentum is given by $(m, n, o) = (\rho u, \rho v, \rho w)$ and s_k represents the production of species from chemical reactions. Equations (2.1a) represent continuity of individual species, conservation of momentum and energy, respectively. (The global continuity equation can be determined by adding all the individual species continuity equations.)

2.2 Equation of state

We also assume that the macroscopic, thermodynamic properties of the gas are related through the general equation of state

$$p = p(\rho_1, \rho_2, \ldots, \rho_{ns}, i) \tag{2.2}$$

where i is the specific internal energy, so that the total energy is given by

$$e = \rho i + \tfrac{1}{2}(\rho u^2 + \rho v^2 + \rho w^2) \tag{2.3}$$

We note that for chemical non-equilibrium flows, the value of each ρ_i depends not only on the transport of the fluid, but also on the progress of chemical reactions. Therefore, unlike for equilibrium gases, *a priori* determination of an equation of state is not possible, and the equation of state has to be constructed along with the solution process. It is not our purpose here, however, to make an original contribution to this aspect of the flow calculation and we assume that it is possible to determine the pressure from the equation of state together with the associated partial derivatives

$$p_{\rho_k} = \frac{\partial p}{\partial \rho_k}(\rho_1, \rho_2, \ldots, \rho_{ns}, i)\,|_{i, \rho_j, \quad j=1,ns, \quad j \neq k}$$

$$p_i = \frac{\partial p}{\partial i}(\rho_1, \rho_2, \ldots, \rho_{ns}, i)\,|_{\rho_j, \quad j=1,ns}$$

(i.e. where all other variables are held constant). A particular example of this process can be found in [4].

2.3 Structure

Following [1] on flux-difference splitting for non-equilibrium flows in one dimension, we now note the structure of the Jacobian of the flux function (2.1c), in particular, its eigenvalues and eigenvectors. This is essential to a scheme incorporating numerical characteristic decomposition where an explicit time stepping scheme is applied to each of the scalar problems arising from a 'locally frozen' version of (2.1a), and this process is described more fully in §3. For simplicity, we discuss the case with $ns = 3$, i.e. three species; however, the results are easily generalised.

The eigenvalues of the Jacobian

$$\underset{\sim}{A} = \partial \underset{\sim}{f} / \partial \underset{\sim}{w} \tag{2.4}$$

are given by

$$\lambda_j = u \pm a, u, u, u, u, u, \qquad j = 1, \ldots 7 \tag{2.5a-g}$$

with corresponding eigenvectors

$$\underset{\sim}{e}_{1,2} = (c_1, c_2, c_3, u \pm a, v, w, H \pm ua)^T \tag{2.6a-b}$$

$$\underset{\sim}{e}_3 = \left(1, 0, 0, u, v, w, i + \tfrac{1}{2}q^2 - \frac{\rho p_{\rho_1}}{p_i}\right)^T \tag{2.6c}$$

$$\underset{\sim}{e}_4 = \left(0, 1, 0, u, v, w, i + \tfrac{1}{2}q^2 - \frac{\rho p_{\rho_2}}{p_i}\right)^T \tag{2.6d}$$

$$\underset{\sim}{e}_5 = \left(0, 0, 1, u, v, w, i + \tfrac{1}{2}q^2 - \frac{\rho p_{\rho_3}}{p_i}\right)^T \tag{2.6e}$$

$$\underset{\sim}{e}_6 = (0, 0, 0, 0, 1, 0, v)^T \tag{2.6f}$$

and

$$\underset{\sim}{e}_7 = (0, 0, 0, 0, 0, 1, w)^T \tag{2.6g}$$

where the sound speed a, the enthalpy H and the fluid speed q are given by

$$a^2 = c_1 p_{\rho_1} + c_2 p_{\rho_2} + c_3 p_{\rho_3} + p p_i / \rho^2 \tag{2.7}$$

$$H = p/\rho + i + \tfrac{1}{2}q^2 \tag{2.8}$$

and

$$q^2 = u^2 + v^2 + w^2. \tag{2.9}$$

(N.B. In order to determine the Jacobian in (2.4) it is necessary to calculate the partial derivatives of the equation of state (2.2) (with $ns = 3$) with respect to the conserved variables $\rho_1, \rho_2, \rho_3, m, n, o$ and e. For this we use the chain rule for partial derivatives and the energy relation (2.3) written as

$$i = i(\rho_1, \rho_2, \rho_3, m, n, o, e) = \frac{e}{\rho} - \tfrac{1}{2}\frac{m^2+n^2+o^2}{\rho^2}$$

where

$$\rho = \rho_1 + \rho_2 + \rho_3.$$

Thus

$$\frac{\partial i}{\partial \rho_1}(\rho_1, \rho_2, \rho_3, m, n, o, e) \mid_{\rho_2, \rho_3, m, n, o, e} = -\frac{H}{\rho} + \frac{p}{\rho^2} + \frac{q^2}{\rho},$$

and hence

$$\frac{\partial p}{\partial \rho_1}(\rho_1, \rho_2, \rho_3, i(\rho_1, \rho_2, \rho_3, m, e)) \mid_{\rho_2, \rho_3, m, n, o, e} =$$

$$\frac{\partial p}{\partial \rho_1}(\rho_1, \rho_2, \rho_3, i) \mid_{\rho_2, \rho_3, i} + \frac{\partial p}{\partial i}(\rho_1, \rho_2, \rho_3, i) \mid_{\rho_1, \rho_2, \rho_3} \left(-\frac{H}{\rho} + \frac{p}{\rho^2} + \frac{q^2}{\rho}\right)$$

with similar expressions for $\partial p/\partial \rho_2$ and $\partial p/\partial \rho_3$. Similarly,

$$\frac{\partial p}{\partial m} \mid_{\rho_1, \rho_2, \rho_3, n, o, e} = \frac{\partial p}{\partial i} \mid_{\rho_1, \rho_2, \rho_3} \left(-\frac{u}{\rho}\right)$$

and

$$\frac{\partial p}{\partial e} \mid_{\rho_1, \rho_2, \rho_3, m, n, o} = \frac{\partial p}{\partial i} \mid_{\rho_1, \rho_2, \rho_3} \left(\frac{1}{\rho}\right),$$

and for $\partial p/\partial n \mid_{\rho_1, \rho_2, \rho_3, m, o}$, $\partial p/\partial o \mid_{\rho_1, \rho_2, \rho_3, m, n}$.) Similar expressions for $\underset{\sim}{B} = \partial \underset{\sim}{g}/\partial \underset{\sim}{w}$ and $\underset{\sim}{C} = \partial \underset{\sim}{h}/\partial \underset{\sim}{w}$ can be deduced by symmetry.

In the next section we describe how this structure can be exploited in a Riemann solver for solving equations (2.1a).

3. APPROXIMATE RIEMANN SOLVER

We now present a numerical scheme for the solution of (2.1a) with particular emphasis on the flux term $\underset{\sim}{f}_x$ (and the use of operator splitting) and this will be based on a Riemann solver. The treatment of the source term, however, will generally require a stiff solver and this is not the purpose of this paper. Thus we shall concentrate on obtaining approximate solutions of the homogeneous problem

$$\underset{\sim}{w}_t + \underset{\sim}{f}_x + \underset{\sim}{g}_y + \underset{\sim}{h}_z = \underset{\sim}{0} \tag{3.1}$$

in a time interval Δt. This solution can then be incorporated with an ordinary differential equation solver based on a Runge-Kutta scheme, say, in order to solve the full problem (2.1a), (see §3.3).

3.1 Operator Splitting

We seek to solve equation (3.1) (and hence the corresponding inhomogeneous equation (2.1a)) approximately using the technique of operator splitting [3], i.e. solve successively

$$\underset{\sim}{w}_t + \underset{\sim}{f}_x = \underset{\sim}{0} \tag{3.2a}$$

$$\underset{\sim}{w}_t + \underset{\sim}{g}_y = \underset{\sim}{0} \tag{3.2b}$$

and

$$\underset{\sim}{w}_t + \underset{\sim}{h}_z = \underset{\sim}{0} \tag{3.2c}$$

along x-, y- and z- coordinate lines, respectively. We shall discuss the solution of (3.2a), and the solution of (3.2b-c) will follow by symmetry.

3.2 Linearised Riemann Problem

If the solution of (3.2a) is sought along an x- coordinate line ($y = y_0, z = z_0$) using a finite difference method then the solution is known at a set of discrete mesh points $(x, y, z, t) = (x_j, y_0, z_0, t_n)$ at any time t_n. Following Godunov [5] the approximate solution $\underset{\sim}{w}_j^n$ to $\underset{\sim}{w}$ at (x_j, y_0, z_0, t_n) can be considered as a set of piecewise constants $\underset{\sim}{w} = \underset{\sim}{w}_j^n$ for $x \in \left(x_j - \frac{\Delta x}{2}, x_j + \frac{\Delta x}{2}\right)$ at time t_n, where $\Delta x = x_j - x_{j-1}$ is a constant mesh spacing. A Riemann problem is now present at each interface $x_{j-\frac{1}{2}} = \frac{1}{2}(x_{j-1} + x_j)$ seperating adjacent states $\underset{\sim}{w}_{j-1}^n$, $\underset{\sim}{w}_j^n$. We consider solving the linearised Riemann problem

$$\underset{\sim}{w}_t + \underset{\sim}{\tilde{A}}\left(\underset{\sim}{w}_{j-1}^n, \underset{\sim}{w}_j^n\right) \underset{\sim}{w}_x = \underset{\sim}{0} \tag{3.3}$$

as a means of solving (3.2a) in a time interval $\Delta t = t_{n+1} - t_n$, where $\underset{\sim}{\tilde{A}}_{j-\frac{1}{2}} = \underset{\sim}{\tilde{A}}\left(\underset{\sim}{w}_{j-1}^n, \underset{\sim}{w}_j^n\right)$ is an approximation to the Jacobian $\underset{\sim}{A}$ and is a constant matrix depending on the states either side of $x_{j-\frac{1}{2}}$. The matrix $\underset{\sim}{\tilde{A}}_{j-\frac{1}{2}}$ will be required to satisfy the following properties

(1) $\underset{\sim}{\tilde{A}}_{j-\frac{1}{2}}$ has seven linearly independent eigenvectors (in the case $ns = 3$) and

(2) $\Delta \underset{\sim}{f} = \underset{\sim}{\tilde{A}}_{j-\frac{1}{2}} \Delta \underset{\sim}{w}$.

These properties were shown by Roe [6] in the case of compressible flow of an ideal gas to guarantee conservation and have good shock-capturing properties. These properties were used to construct a scheme for the one-dimensional equations of non-equilibrium flow [1] and the scheme here represents a generalisation of this.

3.3 Numerical Scheme

Once such a matrix has been constructed equation (3.3) can be solved approximately as

$$\frac{\underset{\sim}{w}_k^{n+1} - \underset{\sim}{w}_k^n}{\Delta t} + \underset{\sim}{\tilde{A}}_{j-\frac{1}{2}} \frac{\left(\underset{\sim}{w}_j^n - \underset{\sim}{w}_{j-1}^n\right)}{\Delta x} = \underset{\sim}{0} \tag{3.4}$$

where k can be $j-1$ or j, $\Delta t = t_{n+1} - t_n$ is a constant time step, although this restriction could easily be lifted. If we project

$$\Delta \underset{\sim}{w} = \underset{\sim}{w}_j^n - \underset{\sim}{w}_{j-1}^n = \sum_{i=1}^{7} \tilde{\alpha}_i \tilde{\underset{\sim}{e}}_i, \tag{3.5}$$

where $\tilde{\underset{\sim}{e}}_i$ are the eigenvectors of $\tilde{\underset{\sim}{A}}_{j-\frac{1}{2}}$, then equation (3.4) can be written as

$$\frac{\underset{\sim}{w}_k^{n+1} - \underset{\sim}{w}_k^n}{\Delta t} + \frac{\sum_{i=1}^{7} \tilde{\lambda}_i \tilde{\alpha}_i \tilde{\underset{\sim}{e}}_i}{\Delta x} = \underset{\sim}{0} \tag{3.6}$$

where $\tilde{\lambda}_i$ are the eigenvalues of $\tilde{\underset{\sim}{A}}_{j-\frac{1}{2}}$. Equation (3.6) now gives rise to the following first order upwind algorithm along the x- coordinate line $y = y_0$, $z = z_0$

$$\underset{\sim}{w}_{j-1}^{n+1} = \underset{\sim}{w}_{j-1}^n - \frac{\Delta t}{\Delta x} \tilde{\lambda}_i \tilde{\alpha}_i \tilde{\underset{\sim}{e}}_i \qquad \text{if} \quad \tilde{\lambda}_i < 0 \tag{3.7a}$$

or

$$\underset{\sim}{w}_j^{n+1} = \underset{\sim}{w}_j^n - \frac{\Delta t}{\Delta x} \tilde{\lambda}_i \tilde{\alpha}_i \tilde{\underset{\sim}{e}}_i \qquad \text{if} \quad \tilde{\lambda}_i > 0. \tag{3.7b}$$

A similar argument applies for updating in the y- and z- directions, i.e. solving (3.2a-b). The approximate solution $\underset{\sim}{w}_j$ of equation (3.1) at time t_{n+1}, together with the approximate solution of (2.1a) at previous time levels, can be used to find the solution of (2.1a) at t_{n+1} using an appropriate treatment of the source term. A standard fourth order Runga-Kutta scheme for the inhomogeneous equations (2.1a) incorporating the above numerical scheme would be

$$\underset{\sim}{w}^{n+1} = \underset{\sim}{w}^n + \delta \underset{\sim}{w} + \frac{\Delta t}{6} \left(\underset{\sim}{s}^n + 2\, {}^1\underset{\sim}{s}^n + 2\, {}^2\underset{\sim}{s}^n + {}^3\underset{\sim}{s}^n \right),$$

where

$$\begin{aligned} {}^1\underset{\sim}{s}^n &= \underset{\sim}{s}({}^1\underset{\sim}{w}^n), & {}^1\underset{\sim}{w}^n &= \underset{\sim}{w}^n + \tfrac{1}{2}\Delta t\, \underset{\sim}{s}^n, \\ {}^2\underset{\sim}{s}^n &= \underset{\sim}{s}({}^2\underset{\sim}{w}^n), & {}^2\underset{\sim}{w}^n &= \underset{\sim}{w}^n + \tfrac{1}{2}\Delta t\, {}^1\underset{\sim}{s}^n, \\ {}^3\underset{\sim}{s}^n &= \underset{\sim}{s}({}^3\underset{\sim}{w}^n), & {}^3\underset{\sim}{w}^n &= \underset{\sim}{w}^n + \Delta t\, {}^2\underset{\sim}{s}^n. \end{aligned}$$

and $\delta \underset{\sim}{w}$ denotes the increment to $\underset{\sim}{w}^n$ in a time step Δt as a result of applying the numerical scheme above to equations (3.2a-c).

We note here that in order to avoid entropy violating solutions, i.e. expansion shocks, the first order scalar upwind scheme implied by (3.7a-b) can easily be modified [7].

3.4 Construction of $\tilde{\underset{\sim}{A}}_{j-\frac{1}{2}}$

Our aim now is to construct a matrix $\tilde{\underset{\sim}{A}}_{j-\frac{1}{2}} = \tilde{\underset{\sim}{A}}(\underset{\sim}{w}_L, \underset{\sim}{w}_R)$ satisfying properties (1) and (2) of §3.2, where $\underset{\sim}{w}_L, \underset{\sim}{w}_R$ denote $\underset{\sim}{w}_{j-1}^n, \underset{\sim}{w}_j^n$, respectively, and this will be a more general form of the matrix found in [1]. Following the approach in [1] this is equivalent to finding average eigenvalues $\tilde{\lambda}_i$ and average eigenvectors $\tilde{\underset{\sim}{e}}_i$ of the eigenvalues and eigenvectors of the Jacobian $\underset{\sim}{A}$ at x_L, x_R given by equations (2.5a)–(2.6g) such that

$$\Delta \underset{\sim}{w} = \sum_{i=1}^{7} \tilde{\alpha}_i \tilde{\underset{\sim}{e}}_i \tag{3.8a-g}$$

and

$$\Delta \underset{\sim}{f} = \sum_{i=1}^{7} \tilde{\lambda}_i \tilde{\alpha}_i \tilde{\underset{\sim}{e}}_i \tag{3.9a-g}$$

for some wavestrengths $\tilde{\alpha}_i$, where $\Delta(\cdot) = (\cdot)_R - (\cdot)_L$. The form for these wavestrengths is determined by solving (3.8a-g) to within $O(\Delta^2)$ for two close states $\underset{\sim}{w}_L, \underset{\sim}{w}_R$. After some detailed algebra we find that the required solution is

$$\alpha_{1,2} = \frac{1}{2a^2}(\Delta p \pm \rho a \Delta u), \tag{3.10a-b}$$

$$\alpha_3 = \Delta\rho_1 - c_1\frac{\Delta p}{a^2}, \tag{3.10c}$$

$$\alpha_4 = \Delta\rho_2 - c_2\frac{\Delta p}{a^2}, \tag{3.10d}$$

$$\alpha_5 = \Delta\rho_3 - c_3\frac{\Delta p}{a^2}, \tag{3.10e}$$

$$\alpha_6 = \rho\Delta v \tag{3.10f}$$

and

$$\alpha_7 = \rho\Delta w. \tag{3.10g}$$

We now consider two general states $\underset{\sim}{w}_L$, $\underset{\sim}{w}_R$ and solve (3.8a)–(3.9g) exactly where

$$\tilde{\lambda}_i = \tilde{u} \pm \tilde{a}, \tilde{u}, \tilde{u}, \tilde{u}, \tilde{u}, \tilde{u} \tag{3.11a-e}$$

$$\underset{\sim}{\tilde{e}}_{1,2} = \left(\tilde{c}_1, \tilde{c}_2, \tilde{c}_3, \tilde{u} \pm \tilde{a}, \tilde{v}, \tilde{w}, \frac{\tilde{p}}{\tilde{\rho}} + \tilde{i} + \tfrac{1}{2}\tilde{q}^2\right)^T \tag{3.12a-b}$$

$$\underset{\sim}{\tilde{e}}_3 = \left(1, 0, 0, \tilde{u}, \tilde{v}, \tilde{w}, \tilde{i} + \tfrac{1}{2}\tilde{q}^2 - \frac{\tilde{\rho}\tilde{p}_{\rho_1}}{\tilde{p}_i}\right)^T \tag{3.12c}$$

$$\underset{\sim}{\tilde{e}}_4 = \left(0, 1, 0, \tilde{u}, \tilde{v}, \tilde{w}, \tilde{i} + \tfrac{1}{2}\tilde{q}^2 - \frac{\tilde{\rho}\tilde{p}_{\rho_2}}{\tilde{p}_i}\right)^T \tag{3.12d}$$

$$\underset{\sim}{\tilde{e}}_5 = \left(0, 0, 1, \tilde{u}, \tilde{v}, \tilde{w}, \tilde{i} + \tfrac{1}{2}\tilde{q}^2 - \frac{\tilde{\rho}\tilde{p}_{\rho_3}}{\tilde{p}_i}\right)^T \tag{3.12e}$$

$$\underset{\sim}{\tilde{e}}_6 = (0, 0, 0, 0, 1, 0, \tilde{v})^T \tag{3.12f}$$

$$\underset{\sim}{\tilde{e}}_7 = (0, 0, 0, 0, 0, 1, \tilde{w})^T \tag{3.12g}$$

$$\tilde{\alpha}_{1,2} = \frac{1}{2\tilde{a}^2}(\Delta p \pm \tilde{\rho}\tilde{a}\Delta u) \tag{3.13a-b}$$

$$\tilde{\alpha}_3 = \Delta\rho_1 - \tilde{c}_1\frac{\Delta p}{\tilde{a}^2} \tag{3.13c}$$

$$\tilde{\alpha}_4 = \Delta\rho_2 - \tilde{c}_2\frac{\Delta p}{\tilde{a}^2} \tag{3.13d}$$

$$\tilde{\alpha}_5 = \Delta\rho_3 - \tilde{c}_3\frac{\Delta p}{\tilde{a}^2} \tag{3.13e}$$

$$\tilde{\alpha}_6 = \tilde{\rho}\Delta v \tag{3.13f}$$

$$\tilde{\alpha}_7 = \tilde{\rho}\Delta w \tag{3.13g}$$

and

$$\tilde{a}^2 = \tilde{c}_1\tilde{p}_{\rho_1} + \tilde{c}_2\tilde{p}_{\rho_2} + \tilde{c}_3\tilde{p}_{\rho_3} + \frac{\tilde{p}\tilde{p}_i}{\tilde{\rho}^2}, \tag{3.14}$$

and for convenience we have written

$$\tilde{q}^2 = \tilde{u}^2 + \tilde{v}^2 + \tilde{w}^2. \tag{3.15}$$

The derivation of the solution to this problem is quite detailed and thus we only present the final result in terms of the cell averages for $\tilde{c}_1, \tilde{c}_2, \tilde{c}_3, \tilde{\rho}, \tilde{u}, \tilde{v}, \tilde{w}, \tilde{p}, \tilde{p}_{\rho_1}, \tilde{p}_{\rho_2}, \tilde{p}_{\rho_3}, \tilde{p}_i$ and $\tilde{i}$, where $\tilde{a}, \tilde{q}$ are calculated from (3.14) and (3.15). The required values are

$$\tilde{N} = \frac{\sqrt{\rho_L}N_L + \sqrt{\rho_R}N_R}{\sqrt{\rho_L} + \sqrt{\rho_R}}, \qquad N = c_1, c_2, c_3, u, v, w, i \quad \text{and} \quad H \tag{3.16a-h}$$

and

$$\tilde{\rho} = \sqrt{\rho_L \rho_R} \tag{3.17}$$

and where $\tilde{p}$ is calculated from

$$\tilde{p} = \tilde{\rho}(\tilde{H} - \tfrac{1}{2}\tilde{q}^2 - \tilde{i}). \tag{3.18}$$

These are all consistent with those averages found in [1] if the flow has slab symmetry, i.e. $v \equiv w \equiv 0$; otherwise averages are now found for v, w, and more expressions involving $\tilde{q}$ instead of $\tilde{u}$. One consequence of the averages in (3.16a-c) is that

$$\tilde{c}_1 + \tilde{c}_2 + \tilde{c}_3 = 1, \tag{3.19}$$

i.e. the relation $c_1 + c_2 + c_3 = 1$ is satisfied by the average species mass fractions. The corresponding results for the matrices $\tilde{\underset{\sim}{B}}$ and $\tilde{\underset{\sim}{C}}$ can be deduced by symmetry.

Finally, it is necessary to specify the averages for the derivatives of the equation of state, and these are a consequence of (3.9d) which gives

$$\Delta p = \tilde{p}_{\rho_1} \Delta\rho_1 + \tilde{p}_{\rho_2} \Delta\rho_2 + \tilde{p}_{\rho_3} \Delta\rho_3 + \tilde{p}_i \Delta i. \tag{3.20}$$

Restating the results in [1] for completeness we have the solution

$$\tilde{p}_i = \begin{cases} \dfrac{1}{2\Delta i}\left[(p(\underset{\sim}{X}_R, i_R) - p(\underset{\sim}{X}_R, i_L)) \right. \\ \qquad\qquad \left. + (p(\underset{\sim}{X}_L, i_R) - p(\underset{\sim}{X}_L, i_L))\right] & \Delta i \neq 0 \\ \dfrac{1}{2}\left[p_i(\underset{\sim}{X}_R, i) + p_i(\underset{\sim}{X}_L, i)\right], & \Delta i = 0, \quad i_L = i_R = i \end{cases} \tag{3.21a-b}$$

and

$$\tilde{p}_{\rho_1} = \begin{cases} \dfrac{1}{2\Delta\rho_1}\left[(p(\rho_{1_R}, \underset{\sim}{Y}_R) - p(\rho_{1_L}, \underset{\sim}{Y}_R)) \right. \\ \qquad\qquad \left. + (p(\rho_{1_R}, \underset{\sim}{Y}_L) - p(\rho_{1_L}, \underset{\sim}{Y}_L))\right] & \Delta\rho_1 \neq 0 \\ \dfrac{1}{2}\left[p_{\rho_1}(\rho_1, \underset{\sim}{Y}_R) + p_{\rho_1}(\rho_1, \underset{\sim}{Y}_L)\right], & \Delta\rho_1 = 0, \quad \rho_{1_L} = \rho_{1_R} = \rho_1 \end{cases} \tag{3.21c-d}$$

with similar expressions for $\tilde{p}_{\rho_2}$, $\tilde{p}_{\rho_3}$, and where $\underset{\sim}{X} = (\rho_1, \rho_2, \rho_3)$, $\underset{\sim}{Y} = (\rho_2, \rho_3, i)$. The corresponding results found in equations (3.11a)–(3.21d) for more than three species can easily be deduced.

Thus, with the procedure outlined in §3.3, together with the averages determined above, we have generalised the scheme in [1] to treat three-dimensional flows with the aid of operator splitting. To complete the scheme a stiff ordinary differential equation solver is required, which could depend on the nature of the source term $\underset{\sim}{s}$ in (2.1a).

In the next section we propose alternative forms for the approximations in (3.20a-3.21b) which will lead to a more efficient and more robust algorithm.

4. A MODIFIED SCHEME

In this section an alternative pair of averages to (3.21a-d) are proposed to complete the Riemann solver of §3.

As stated in §3, in order to complete the Riemann solver it is necessary to determine averages for $\tilde{p}_{\rho_1}, \tilde{p}_{\rho_2}, \tilde{p}_{\rho_3}$ and $\tilde{p}_i$ of the derivatives $p_{\rho_1}, p_{\rho_2}, p_{\rho_3}$ and p_i, and by virtue of (3.9d) these must satisfy (3.20). Although equations (3.21a-d), together with their counterparts for $\tilde{p}_{\rho_2}$ and $\tilde{p}_{\rho_3}$, represent one solution of (3.20), we note that two distinct disadvantages are apparent.

From (3.21a-d) (and their counterparts) we see that, in general, ten seperate function evaluations of the equation of state (2.2) are needed for $\tilde{p}_{\rho_{1,2,3}}$ and $\tilde{p}_i$ ($2ns + 4$ for ns species) which could prove computationally expensive, and the artificial states $(\underset{\sim}{X}_R, i_L)$, $(\underset{\sim}{X}_L, i_R)$, $(\rho_{1_R}, \underset{\sim}{Y}_L)$ and

$(\rho_{1_L}, \underset{\sim}{Y}_R)$ are introduced. On this last point, it may be that the artificially produced states lie outside the range of validity of the equation of state as it is constructed along with the solution process.

Natural approximations to $p_{\rho_1}, p_{\rho_2}, p_{\rho_3}$ and p_i in the interval (x_L, x_R) arising from the scheme of §3 are

$$\hat{p}_{\rho_j} = p_{\rho_j}(\tilde{\underset{\sim}{Z}}) \qquad j = 1,2,3 \tag{4.1a-c}$$

$$\hat{p}_i = p_i(\tilde{\underset{\sim}{Z}}) \tag{4.1d}$$

where

$$\tilde{\underset{\sim}{Z}} = (\tilde{c}_1\tilde{\rho}, \tilde{c}_2\tilde{\rho}, \tilde{c}_3\tilde{\rho}, \tilde{i}). \tag{4.1e}$$

In particular, as a result of the averages (3.16a-c,g) and (3.17), no artificial states are introduced since

$$(\tilde{c}_1\tilde{\rho}, \tilde{c}_2\tilde{\rho}, \tilde{c}_3\tilde{\rho}, \tilde{i}) \in |(\rho_{1_L}, \rho_{1_R})| \times |(\rho_{2_L}, \rho_{2_R})| \times |(\rho_{3_L}, \rho_{3_R})| \times |(i_L, i_R)|,$$

where we have denoted $|(b_L, b_R)| = (b_L, b_R)$ if $b_L \leq b_R$, or $|(b_L, b_R)| = (b_R, b_L)$ if $b_R < b_L$. Unfortunately, (4.1a-d) do not, in general, satisfy (3.20), i.e.

$$\Delta p \neq \hat{p}_{\rho_1}\Delta\rho_1 + \hat{p}_{\rho_2}\Delta\rho_2 + \hat{p}_{\rho_3}\Delta\rho_3 + \hat{p}_i\Delta i. \tag{4.2}$$

However, to first order

$$\Delta p \simeq \hat{p}_{\rho_1}\Delta\rho_1 + \hat{p}_{\rho_2}\Delta\rho_2 + \hat{p}_{\rho_3}\Delta\rho_3 + \hat{p}_i\Delta i, \tag{4.3}$$

i.e.

$$\Delta p = \hat{p}_{\rho_1}\Delta\rho_1 + \hat{p}_{\rho_2}\Delta\rho_2 + \hat{p}_{\rho_3}\Delta\rho_3 + \hat{p}_i\Delta i + O(\Delta^2), \tag{4.4}$$

and hence

$$p^*_{\rho_j} = \frac{\Delta p - \hat{p}_i\Delta i - \hat{p}_k\Delta\rho_k - \hat{p}_\ell\Delta\rho_\ell}{\Delta\rho_j}, \qquad j = 1,2,3 \tag{4.5a-c}$$

$$p^*_i = \frac{\Delta p - \hat{p}_{\rho_1}\Delta\rho_1 - \hat{p}_{\rho_2}\Delta\rho_2 - \hat{p}_{\rho_3}\Delta\rho_3}{\Delta i} \tag{4.5d}$$

represent first order approximations to $p_{\rho_1}, p_{\rho_2}, p_{\rho_3}$ and p_i respectively, where (jkl) is a cyclic permutation of (123), a notation used throughout the rest of the paper. Thus, a weighted mean of the expressions in (4.1a-d) and (4.5a-d) can satisfy (3.20).

To begin with we assume $\Delta\rho_j, \quad \Delta i \neq 0, \quad j = 1,2,3$ and write

$$\tilde{p}_{\rho_j} = \beta_j\hat{p}_{\rho_j} + (1-\beta_j)p^*_{\rho_j}, \qquad j = 1,2,3 \tag{4.6a-c}$$

and

$$\tilde{p}_i = \beta_4\hat{p}_i + (1-\beta_4)p^*_i \tag{4.6d}$$

for some weights $\beta_{1,2,3,4}$. Substituting (4.6a-d) into (3.20) yields $\beta_4 = 3 - \beta_1 - \beta_2 - \beta_3$, so that

$$\begin{aligned}\tilde{p}_{\rho_j} &= \beta_j\hat{p}_{\rho_j} + (1-\beta_j)p^*_{\rho_j} \\ &= \beta_j p_{\rho_j}(\tilde{\underset{\sim}{Z}}) + \frac{1-\beta_j}{\Delta\rho_j}\left(\Delta p - p_i(\tilde{\underset{\sim}{Z}})\Delta i - p_{\rho_k}(\tilde{\underset{\sim}{Z}})\Delta\rho_k - p_{\rho_\ell}(\tilde{\underset{\sim}{Z}})\right) \qquad j = 1,2,3\end{aligned} \tag{4.7a-c}$$

and

$$\tilde{p}_i = (3-\beta_1-\beta_2-\beta_3)\tilde{p}_i(\tilde{\underset{\sim}{Z}}) + \frac{\beta_1+\beta_2+\beta_3-2}{\Delta i}\Big(\Delta p - p_{\rho_1}(\tilde{\underset{\sim}{Z}})\Delta\rho_1 - p_{\rho_2}(\tilde{\underset{\sim}{Z}})\Delta\rho_2 - p_{\rho_3}(\tilde{\underset{\sim}{Z}})\Delta\rho_3\Big) \tag{4.7d}$$

are suitable approximations to employ in the Riemann solver of §3 in the case $\Delta\rho_j, \quad \Delta i \neq 0, \quad j = 1,2,3$. Specifically, (3.20) is satisfied, only two function evaluations (for $\hat{p}_{\rho_1}$ and $\hat{p}_i$) are required for $\tilde{p}_{\rho_1}$ and $\tilde{p}_i$, and no artificial states are introduced. To deduce a form for the unknown weights $\beta_{1,2,3}$ we look at the limits $\Delta\rho_j, \quad \Delta i \to 0, \quad j = 1,2,3$.

From (3.20), if $\Delta\rho_1 \neq 0$ and $\Delta\rho_{2,3}, \quad \Delta i = 0$, then $\tilde{p}_{\rho_1} = \frac{\Delta p}{\Delta\rho_1}$ and any consistent average for $\tilde{p}_{\rho_{2,3}}, \tilde{p}_i$ will suffice, say $\tilde{p}_{\rho_{2,3}} = \hat{p}_{\rho_{2,3}}, \quad \tilde{p}_i = \hat{p}_i$. Thus, in this case from (4.7a-d), we require that $\beta_1 = 0, \quad \beta_2 = \beta_3 = 1$. More generally, as $\Delta\rho_{2,3}, \quad \Delta i \to 0, \quad \Delta\rho_1 \neq 0$, we require (from (4.7a-d)) that $\beta_1 \to 0, \quad \beta_{2,3} \to 1$. Similarly for the other limits, as $\Delta\rho_{k,l}, \quad \Delta i \to 0, \quad \Delta\rho_j \neq 0$ we require that $\beta_1 \to 0, \quad \beta_{k,l} \to 1, \quad j = 1,2,3$; and finally, for $\Delta\rho_{1,2,3} \to 0, \quad \Delta i \neq 0$, we require $\beta_{1,2,3} \to 1$. A set of weights that satisfy these conditions are

$$\beta_j = (|\Delta\rho_k| + |\Delta\rho_\ell| + |\Delta i|)/\sigma, \qquad j = 1,2,3 \tag{4.8a-c}$$

where

$$\sigma = |\Delta\rho_1| + |\Delta\rho_2| + |\Delta\rho_3| + |\Delta i| \tag{4.8d}$$

and hence $\beta_4 = 3-\beta_1-\beta_2-\beta_3 = (|\Delta\rho_1| + |\Delta\rho_2| + |\Delta\rho_3|)/\sigma$, which are particularly simple to compute; however, we note that this choice is not unique. It is then a straightforward matter to check that

$$\lim_{(\Delta\rho_{1,2,3},\Delta i)\to\underset{\sim}{0}} \tilde{p}_{\rho_j} = p_{\rho_j}(\rho_1,\rho_2,\rho_3,i), \qquad j = 1,2,3, \tag{4.9a-c}$$

and

$$\lim_{(\Delta\rho_{1,2,3},\Delta i)\to\underset{\sim}{0}} \tilde{p}_i = p_i(\rho_1,\rho_2,\rho_3,i), \tag{4.9d}$$

using the definitions in (4.1e), (4.7a-d) and (4.8a-d).

For computational purposes, one needs to take care when the relative differences, say $\frac{\Delta\rho_j}{\tilde{\rho}}$ and $\frac{\Delta i}{\tilde{i}}, \quad j = 1,2,3$, are close to the rounding error of the machine. Thus we suggest the following averages for practical use

$$\left.\begin{aligned}\tilde{p}_{\rho_j} &= p_{\rho_j}(\tilde{\underset{\sim}{Z}})\\ \tilde{p}_i &= p_i(\tilde{\underset{\sim}{Z}})\end{aligned}\right\} \text{if} \quad \frac{|\Delta\rho_{1,2,3}|}{\tilde{\rho}} \leq 10^{-m} \quad \text{and} \quad \frac{|\Delta i|}{\tilde{i}} \leq 10^{-m} \qquad j = 1,2,3 \tag{4.10a}$$

$$\left.\begin{aligned}\tilde{p}_{\rho_j} &= \beta_j p_{\rho_j}(\tilde{\underset{\sim}{Z}}) + (1-\beta_j)\frac{\Big(\Delta p - p_i - p_{\rho_k}(\tilde{\underset{\sim}{Z}})\Delta\rho_k - p_{\rho_\ell}(\tilde{\underset{\sim}{Z}})\Delta\rho_\ell\Big)}{\Delta\rho_j} \quad j = 1,2,3,\\ \tilde{p}_i &= \beta_4 p_i(\tilde{\underset{\sim}{Z}}) + (1-\beta_4)\frac{\Big(\Delta p - p_{\rho_1}(\tilde{\underset{\sim}{Z}})\Delta\rho_1 - p_{\rho_2}(\tilde{\underset{\sim}{Z}})\Delta\rho_2 - p_{\rho_3}(\tilde{\underset{\sim}{Z}})\Delta\rho_3\Big)}{\Delta i}\end{aligned}\right\} \text{otherwise} \tag{4.10b}$$

where m is machine dependent, and the β_j are as before.

Finally, we note the rearrangement of (4.10b) gives

$$\left.\begin{aligned}\tilde{p}_{\rho_j} &= p_{\rho_j}(\tilde{\underset{\sim}{Z}}) + \frac{|\Delta\rho_j|}{\sigma}\frac{\delta p}{\Delta\rho_j}, \qquad j = 1,2,3,\\ \tilde{p}_i &= p_i(\tilde{\underset{\sim}{Z}}) + \frac{|\Delta i|}{\sigma}\frac{\delta p}{\Delta i},\end{aligned}\right\} \tag{4.10c}$$

where $\tilde{\underset{\sim}{Z}}$ and σ are as before (see (4.1e) and (4.8d)) and where

$$\delta p = \Delta p - p_{\rho_1}(\tilde{\underset{\sim}{Z}})\Delta\rho_1 - p_{\rho_2}(\tilde{\underset{\sim}{Z}})\Delta\rho_2 - p_{\rho_3}(\tilde{\underset{\sim}{Z}})\Delta\rho_3 - p_i(\tilde{\underset{\sim}{Z}})\Delta i, \tag{4.10d}$$

representing the discrepancy in the inequality (4.2). It is the form in (4.10a,c,d) that we propose using in the Riemann solver of §3. Importantly, the averages satisfy the required necessary condition (3.20), only four function evaluations are required for $\tilde{p}_{\rho_{1,2,3}}$ and $\tilde{p}_i$, compared with ten previously. With ns species, $ns+1$ function evaluations are required, compared with $2ns+4$. This clearly optimises the number of function calls since we need approximations to the $ns+1$ derivatives $p_{\rho_{1,2\ldots ns}}, p_i$.

Comparing the c.p.u. time used using an Amdahl V7 we find that for 1 species, an ideal gas equation of state and a second order scheme, the original scheme takes 0.00178 c.p.u. seconds per cell, whereas the modified scheme takes 0.00142 c.p.u. seconds per cell. This represents a significant improvement, which increases further with more species and more complicated equations of state.

5. CONCLUSION

We have extended the scheme in [1] to treat three-dimensional, non-equilibrium flows using operator splitting. This includes the more general flux terms and the corresponding larger set of eigenvalues and eigenvectors required for the algorithm. It is then a straightforward matter to extend existing codes to treat two- or three-dimensional flows. We have also made a significant improvement in the efficiency and robustness of the original scheme. This has been achieved by using alternative averages for the derivatives of the equation of state, and the shock-capturing property guaranteed by equations (3.8a)–(3.9g) is maintained. Again, existing one-dimensional codes can be easily altered to incorporate this modification.

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